

## **THEORETICAL PHYSICS DIVISION**

Ph. D. Branko Guberina, Head of the Division

Programme (until 30<sup>th</sup> june 2002):

### **THEORETICAL RESEARCH OF THE STRUCTURE OF THE MATTER**

Head of the Programme: Ph. D. Branko Guberina

#### **Research programme:**

Presently, the research performed in the Division is mainly theoretical high-energy physics (particle physics, general and mathematical physics, astroparticle physics and cosmology) and condensed matter. Recently, one of the groups has started a new activity by applying linear and nonlinear dynamics analysis to various biomedical problems to study the presence of chaotic behavior and fractal structure.

From the very beginning, members of the Division have lectured at undergraduate and postgraduate studies at the universities in Croatia, mostly at the University of Zagreb. A number of students presently perform their B. Sc., M. Sc., and Ph. D. theses. The Division numbers presently 17 scientists and 15 students and postdocs.

Projects:

#### **PHYSICS OF SURFACES, MICROSTRUCTURES AND STRONGLY CORRELATED SYSTEMS**

Head of the Project: Ph. D. Radovan Brako

#### **FUNDAMENTAL INTERACTIONS IN ELEMENTARY PARTICLE PHYSICS AND COSMOLOGY**

Head of the Project: Ph. D. Branko Guberina

#### **QUANTUM FIELD THEORY, NONCOMMUTATIVE SPACES, AND SYMMETRIES**

Head of the Project: Ph. D. Stjepan Meljanac

#### **STRUCTURE OF DYNAMICAL FLUCTUATIONS IN NONLINEAR SYSTEMS**

Head of the Project: Ph. D. Mladen Martinis

#### **NONLINEARITY AND DETERMINISTIC CHAOS IN CARDIOLOGY**

Head of the Project: Ph. D. Mladen Martinis

## **DIVISION OF EXPERIMENTAL PHYSICS**

Ph. D. Ante Ljubičić, Head of the Division

Programme (until 30<sup>th</sup> june 2002):

### **INVESTIGATIONS IN SUBATOMIC PHYSICS**

Head of the Programme: Ph. D. Ante Ljubičić

#### **Research programme and results:**

In the experiments with stable and radioactive beams numerous reactions between light nuclei have been measured in order to study these processes and the structure of light nuclei in the states at high excitations (especially by searching for exotic phenomena) as well as to obtain data important to nuclear astrophysics. Validity of

different approximations to the postform DWBA transition amplitude for the Coulomb break-up of neutron halo nuclei has been studied.

The Crystal Ball collaboration has finished collecting data for AGS E958 experiment (Pion Charge Exchange Cross Sections at Low Energies), which studies nucleon and its excited states by measuring cross section and angular distribution of  $\pi\text{-p}\rightarrow\pi^0\text{n}$  reaction in momentum range of 50 – 180 MeV/c. The data analyses of this experiment and previously done BNL experiments (E913, E914 and E897) are underway. We are continuing active participation in Baryon Resonance Analysis Group (BRAG). Our partial wave analysis model of meson-nucleon scattering amplitudes has become universally acknowledged in scientific community.

Heavy-ion collisions have been investigated in a broad range of energies and for various projectile-target pairs. At low energies the importance of the alpha-particle exchange process for the proper description of carbon and oxygen reactions has been shown and a clear indication of the formation of the strongly deformed high-spin states of  $^{40}\text{Ca}$  in the  $^{12}\text{C} + ^{28}\text{Si}$  reaction has been found. At higher energies (400 AMeV) lack of the full particle mixing and partial nuclear transparency has been found by analysing all four colliding systems of  $^{96}\text{Zr}$  and  $^{96}\text{Ru}$ , the nuclei of the same mass number but of different isospin. Comparison of the obtained experimental results with the theoretical predictions of the microscopic transport calculation do not require a modification of the free nucleon-nucleon cross section in nuclear medium. Additional data on the nucleon-nucleon cross section have been obtained by measuring with high statistics the very small cross sections of two-photon and virtual bremsstrahlung from proton-proton scattering at 190 MeV.

In 2002 we were involved in the investigation of the trial RPC detectors of large dimensions (cc. 5m x 1 m) that are supposed to be built in the muon spectrometer detector of the OPERA experiment placed at the Gran Sasso tunnel near Rome. We have also participated in the CAST experiment at CERN, which is designed to search for solar axions. We have participated in the development of the TPC detector as well as in the development of data acquisition system. At the Laboratory for Electromagnetic and Weak Interactions we have started the construction of a new system for detection of hadronic axions emitted from the Sun in the M1 transition between first excited 9.3 keV and ground state in  $^{83}\text{Kr}$ .

We have found interesting new bounds for possible contribution of “quintessence” to violation of the Equivalence Principle, both in the sector of ordinary matter and neutrinos. In some cases, our bounds are even better than the limits from present experimental data on the universality of the free fall. The consistently coupled Schwinger-Dyson and Bethe-Salpeter equations are solved for  $\eta - \eta'$  complex.

Results for the two-photon transitions are calculated and compared with the experiment.

Correlations in high-energy atomic processes, including photoabsorption, photon scattering and scattering of charged particles, is studied. A new covariant formulation of the relativistic electrodynamics is proposed.

Interactions of ion beams of MeV energy range have been studied in two main directions. The first one has been research of the basic properties of ion beam interactions with atoms (ionization of inner shells) and nuclei (elastic and inelastic scattering). The second direction has been development and application of ion beam techniques for the material characterization and modifications. The most significant was development of IBIC (Ion Beam Induced Charge) technique that has been applied in studies of charge transport properties at microscopic level in different wide gap semiconductors.

Monitoring of isotopes  $^{14}\text{C}$  and  $^3\text{H}$  in the atmosphere was continued in order to study their natural cycle in the environment and to assess paleoclimatic condition in Dinaric Karst. Isotopic measurements ( $^3\text{H}$ ,  $^2\text{H}$ ,  $^{18}\text{O}$ ) in precipitation were extended to the Adriatic region. Optimal conditions for  $^{14}\text{C}$  and  $^3\text{H}$  measurements in liquid scintillation

counter (LSC) were established. For  $^{14}\text{C}$  dating method in LSC the procedure of sample preparation by direct absorption method was developed and a new vacuum rig for benzene preparation was constructed and tested. Radiocarbon dating of several archaeological and geological series from different sites in Croatia and Slovenia was performed.

Pp, pA and AA data was analysed at SpS energies of 40-160 GeV/nucleon at the CERN NA49 experiment. Detailed energy dependence of the charged particle production (pions, protons, kaons) as well as of the production of strange hyperons (Lambda, Xi, Omega) was arrived at. These results, together with the results from the other heavy ion experiments at CERN provide a strong indication for the discovery of quark-gluon plasma in a laboratory environment.

Possibilities of using 14 MeV neutron induced (n;n'gamma) reactions, with associated alpha particle detection, for threat material (explosives in the first place) identification have been investigated. Characterization of soil samples taken from mine affected areas has been performed. Measurements of small scale variations of soil humidity have determined the limits of applicability of some nuclear methods for detection of AP and AT landmines.

#### Projects:

##### **HADRONIC PHYSICS AND QCD**

Head of the Project: Ph. D. Ivan Supek

##### **LIGHT ATOMIC NUCLEI: CLUSTERS, NUCLEAR MOLECULES, REACTIONS**

Head of the Project: Ph. D. Đuro Miljanić

##### **INTERACTIONS IN SUBATOMIC AND MEDICAL PHYSICS**

Head of the Project: Ph. D. Alfred Švarc

##### **HEAVY-ION PHYSICS**

Head of the Project: Ph. D. Zoran Basrak

##### **MASSIVE NEUTRINOS AND ASTRO-PARTICLES**

Head of the Project: Ph. D. Ante Ljubičić

##### **PHOTON ATOM INTERACTIONS AND CORRELATIONS**

Head of the Project: Ph. D. Tihomir Surić

##### **PROCESSES OF FAST ION INTERACTIONS WITH MATTER**

Head of the Project: Ph. D. Milko Jakšić

##### **NATURAL ISOTOPES OF WEAK ACTIVITIES AND DEVELOPMENT OF INSTRUMENTATION**

Head of the Project: Ph. D. Bogomil Obelić

##### **HIGH-ENERGY EXPERIMENTAL PHYSICS**

Head of the Project: Ph. D. Krešo Kadija

##### **METHODS OF EXPLOSIVE, CHEMICAL AND NUCLEAR MATERIAL DETECTION**

Head of the Project: Ph. D. Vladivoj Valković

##### **INVARIANT SPECIAL RELATIVITY AND ELECTRODYNAMICS**

Head of the Project: Ph. D. Tomislav Ivezić

## **DIVISION OF MATERIALS PHYSICS**

Ph. D. Branko Pivac, Head of the Division

Programme (until 30<sup>th</sup> June 2002):

### **STUDY OF DEFECTS DISORDERED/ORDERED MATTER AND MOLECULES; INTERACTIONS AND DYNAMICS**

Head of the Programme: Ph. D. Branko Pivac

#### **Research programme:**

Research programme is focussed on following subjects:

- study of fundamental characteristics of defects, their mutual interaction, as well as their impact on connection between microscopic and macroscopic properties of materials in simple (Si), binary (GaAs, GaN, CdS), and multinary semiconductors and complementary oxides. Study of nanophase and glassy material characteristics.
- study of amorphous thin films produced by non-equilibrium thermodynamical processes (magnetron sputtering). Particularly Al-W and WC films will be studied. Processes in plasma obtained during laser ablation of metallic and non-metallic materials will be studied.
- fundamental research in the field of molecular and solid state physics with special emphasis on vibrational spectroscopy. The systems under investigation vary in their origin and composition - from metals, semiconductors, and ceramics on one side to molecular crystals and biological samples on the other.

Projects:

#### **MULTYPHASE AMORPHOUS SILICON ALLOYS AS A THIN FILMS**

Head of the Project: Ph. D. Davor Gracin

#### **SUGAR HYDRATION DYNAMICS**

Head of the Project: Ph. D. Vlasta Mohaček Grošev

#### **IMPACT OF DEFECTS AND NANOSTRUCTURES ON SEMICONDUCTOR PROPERTIES**

Head of the Project: Ph. D. Branko Pivac

#### **MAGNETRON DEPOSITION OF THIN FILMS**

Head of the Project: dr.sc. Nikola Radić

#### **PHYSICS AND APPLICATION OF NANOSTRUCTURES**

Head of the Project: Ph. D. Krešimir Furić

#### **NANOPHASE FILMS AND NANOCOMPOSITE SOLID ELECTROLYTES RESEARCH**

Head of the Project: Ph. D. Aleksandra Turković

#### **STRUCTURE AND ELECTRICAL RELAXATION IN GLASSES AND GLASS- CERAMICS**

Head of the Project: Ph. D. Andrea Moguš-Milanković

#### **STATICS AND DYNAMICS OF MOLECULAR SOLIDS**

Head of the Project: Ph. D. Davor Kirin

## **OPTICAL INTERACTIONS AND ORGANIZATIONAL PROCESSES IN MATTER**

Head of the Project: Ph. D. Stjepan Lugomer

## **SEMICONDUCTOR MATERIALS FOR OPTOELECTRONICS**

Head of the Project: Ph. D. Branko Šantić

## **DIVISION OF ELECTRONICS**

Ph. D. Božidar Vojnović, Head of the Division

Programme (until 30<sup>th</sup> june 2002):

### **PROCESS MODELLING BY INTELLIGENT COMPUTER SYSTEMS**

Head of the Programme: Ph. D. Nikola Bogunović

#### **Research programme:**

The programme strives to investigate and develop modelling, optimisation and automated diagnostic procedures of technical processes by intelligent computer systems. Prerequisites for optimal process modelling are first-rate primary signal processing methods that build upon the classical deterministic and stochastic techniques, and aspire to enhance these methods by employing artificial neural networks and genetic algorithms. The presumption on probabilistic features of signals includes inherent process characteristics and all perturbations in its amplitude (energy) and time domain. Process model construction are based on automated inductive procedures that discover relations within the measured or simulated data sets. Automated model-based reasoning continue to employ symbolic logic and theorem proving methods, augmented with fuzzy variables, uncertainty measures, probabilistic causal networks and case-based reasoning. Special attention is paid to contemporary adaptive modelling of 3D visual user interfaces. The research on this programme generated several refined and new optimisation, predictive and diagnostic procedures, as well as new computer architectures that support advanced embedded process modelling.

Projects:

### **AUTOMATED KNOWLEDGE DISCOVERY AND REASONING**

Head of the Project: Ph. D. Nikola Bogunović

### **ANALYSIS OF STOCHASTIC SIGNALS, TIME SERIES AND DATA STRUCTURES**

Head of the Project: Ph. D. Božidar Vojnović

### **DETEKCTION OF NON-STATIONARY SOURCES AND DISTRIBUTED INFORMATION PROCESSING**

Head of the Project: Ph. D. Karolj Skala

## **DIVISION OF PHYSICAL CHEMISTRY**

Ph. D. Leo Klasinc, Head of the Division

Programme (until 30<sup>th</sup> june 2002):

## STRUCTURE AND DYNAMICS OF SYNTHETIC AND BIOLOGICAL SUBSTANCES

Head of the Programme: Ph. D. Nenad Trinajstić

### Research programme:

Division of Physical Chemistry has expertise and exceptional research productivity in structural chemistry, theoretical chemistry, spectroscopy, atmospheric chemistry, chemical kinetics, modelling of substance properties and both physical and chemical processes, risk assessment, structural and chemical analyses. Furthermore, several research teams have also applied their expertise and extended their research activities into various areas of biosciences.

Current research in atmospheric chemistry involves investigation of trace constituents of air, their properties, transformation and transport in the atmosphere over the different regions of Croatia: continental remote regions and coastal areas. Structural, kinetic and thermodynamic properties are investigated for compounds that enter the atmosphere and contribute in air-soil and air-water exchange. Continuous efforts are made to study homogeneous chemical reactions with an unknown reaction mechanism in liquid and gaseous phase and heterogeneous reactions in gas/solid and gas/liquid phases which are very important for biological activity, chemical production and environmental research. The main aim is to find to what extent a reaction can be guided by changing reaction conditions; in other words, which part depends exclusively on the reactants. An example of such study is the investigation on properties and reactions of natural compounds radical anions with antioxidant property (especially flavonoids) and the attempt to explain their antioxidant activity through quantum chemical calculations. A powerful combination of photoelectron spectroscopy and quantum chemical calculations has been used to resolve electronic structure of small natural products (e.g. sesquiterpenes) and its effect on their physiological activity. In structure-activity relationship studies of biologically active molecules and their analogues, X-ray diffraction analysis, computational chemistry methods, molecular computer graphics, spectroscopic methods and bioassays have been used. Molecular recognition approach, based on the characteristic structural parameters, particularly of the active site or bioactive conformations together with physico-chemical properties of the molecules studied have been used to study biological processes at the molecular level. Molecular modelling, including methods of molecular dynamics which can simulate experimental conditions and/or real parameters *in vivo*, is one of the elements of molecular recognition approach. Molecular dynamics simulations have been used to study conformational stability and substrate binding to the active site of a receptor. The structure-function relationship of human serum lipoproteins is studied by EPR and fluorescence spectroscopy to elucidate the complex structure of these supramolecular assemblies and their functions in the pathology of different diseases (atherosclerosis, diabetes). Liposomes with incorporated drugs are used as a delivery system for pharmacologically active molecules to the targeted cells. The study of physical and chemical nature of interactions of the pharmacologically active molecules, amino acids, peptides and their copper(II) complexes with liposomes is of special interest for development of the efficient delivery methods. EPR spectroscopy was used to study such complex supramolecular systems.

A general mathematical formalism is developed for describing interaction of an arbitrary finite quantum system with an arbitrary finite but known quantum system. This formalism is exact, produces correct results even for strong interaction between the two systems, and can be applied to describe statical and dynamical properties of a system subject to such interaction. This formalism should enable a detailed description of the interaction of a molecule with electromagnetic field, a molecule with the surface or a solid state, a molecule in a solution with the solvent, etc. In the research on the low energy collisions of atom and molecule the potential for Ar-HF

system was investigated since existing data are unreliable. The classical relativistic calculation of dynamics of the electron in the electromagnetic plane wave was investigated, including radiation reaction force. Today, it is feasible to study the ultrafast intramolecular processes and chemical reactions directly by the application of advanced quantum-chemical and quantum-dynamic methods. Ab initio multiconfigurational CASSCF and CASPT2 methods were employed to study the reaction mechanisms and kinetics of the gas-phase ozone additions to ethene, fluoroethene, and chloroethene. We have also investigated the spectroscopy and dynamics of the intramolecular hydrogen bond in malonaldehyde and acetylacetone as well as the specific type of multiresonant laser pulses that can be used to achieve very precise and complete population transfer between two arbitrary states connected by a cascade of dipole transitions in a general quantum system. Algorithm for selection of most important variables/descriptors in linear and nonlinear multiregression models was upgraded, improved and compared with alternative selection methods. Previously developed models for calculation of viscosity and solubility of molecules and for prediction of protein secondary structure content in soluble proteins were significantly simplified and improved. Possibility to optimize topological descriptors was investigated. Basic factors determining structure and properties of fullerenes, nanotubes and similar carbon cages is their topology, i.e. how carbon atoms are connected to build these structures. The topological methods could be also applied to select the most plausible isomers and to determine their geometry. The problem of geometry determination is partially solved by applying the so called AME (Adjacency Matrix Eigenvectors) method. The possibility of numerical characterization of DNA and its segments of chemical and biological interest is examined.

The paramagnetic defects and their usage as paramagnetic probes in the study of dynamics of the crystal lattice of ferroelectric and magnetic systems as well as synthetic macromolecules have been investigated. Electron spin resonance (ESR) method which provides investigation of various types of defects in molecular structures and enables an insight into the dynamics of observed center including surrounding atomic and molecular groups will be used. By using this method a better understanding of microscopic parameters important for the prediction of macroscopic properties of molecular systems with short and long range order will be achieved. The new theoretical model for phase transition, suggested earlier, was employed to better describe microscopic origin of ferroelectric-paraelectric phase transition. The paramagnetic probes were also used to study the motional heterogeneity of segmented polyurethane-polymethacrylate in order to learn more on structural and dynamic heterogeneity of polymers, copolymers, polymer mixtures and interpenetrating polymer networks. The research programme comprises investigations of the novel complex compounds with specific structural and biological properties. Special attention is directed to the study of interactions of alkali and transition metal ions with derivatives of aminophosphonic acids as well as various macrocyclic and heterocyclic compounds, which are used as models for biological and biologically active molecules. The investigations include preparation of the polydentate ligands with N and O donor atoms as well as their complexes, determination of chemical and structural properties of these compounds and studying the mechanism of complexation reactions and stability of complexes in solution, gas and solid phase. The biological properties of ligands and complexes are examined by evaluation of their *in vitro* antitumor and antiviral activity on human and animal cell lines. Research has been continued on complexes of aluminium and silicon with organic ligands of geochemical significance as well as the measurements of total mercury and of methylmercury in the sediments of Kaštela Bay. Trace elements will be determined in sediments and tufa in an effort to better understand their geochemical cycles. The research in chemistry of the surfactants is focused on the relation between surfactant molecular structure and supramolecular organization

(monolayers, micelles, vesicles, lyotropic liquid crystals) in aqueous solutions as well as to determine the structure and thermal phase transitions of surfactant crystals (polymorphism, thermotropic liquid crystals). The research in free radical chemistry covers physico-chemical properties, kinetics and reaction mechanisms of processes involving free radicals and excited molecules. The mobility of essential and toxic metals in plants has been studied on the model systems. Moreover, the Division also provides the following custom services: (i) FT-IR urinary calculi spectroscopic analysis, (ii) organic microanalysis (C, H, N, S, and halogens Cl, Br) and (iii) evaluation of oil spill dispersant efficiency.

In addition to the exceptional research productivity, the Division of Physical Chemistry has contributed extensively to undergraduate as well as to graduate education in Croatia. It has also rich tradition in the organization of international scientific conferences, workshops and summer schools; e.g. 28 conferences organized since 1986. During the last year Division members have provided 32 undergraduate and graduate courses at Universities in Zagreb, Split, Rijeka and Osijek as well as organized two international conferences, the 17<sup>th</sup> MATH/CHEM/COMP in Dubrovnik and the 8<sup>th</sup> Brijuni Conference "Space, Time and Life" at the Brijuni Islands.

#### Projects:

#### **PROPERTIES AND BEHAVIOUR OF ATMOSPHERIC MICROCONSTITUENTS**

Head of the Project: Ph. D. Tomislav Cvitaš

#### **SURFACTANTS, PROCESSES IN SOLUTIONS AND INTERFACES**

Head of the Project: Ph. D. Nada Filipović-Vinceković

#### **REACTIVITY AND REACTION MECHANISMS**

Head of the Project: Ph. D. Leo Klasinc

#### **INVESTIGATION ON CHEMICAL REACTIVITY AND ULTRAFAST PROCESSES**

Head of the Project: Ph. D. Aleksandar Sabljic

#### **DEVELOPMENT AND APPLICATION OF MODELS IN CHEMISTRY AND BIOINFORMATICS**

Head of the Project: akademik Nenad Trinajstić

#### **STRUCTURAL AND BIOLOGICAL INVESTIGATIONS OF NEW COMPLEX COMPOUNDS**

Head of the Project: Ph. D. Ljerka Tušek-Božić

#### **STRUCTURE AND PROPERTIES OF (BIO)MOLECULES**

Head of the Project: Ph. D. Biserka Kojić-Prodić

#### **BIOPHYSICS OF LIPOPROTEIN INTERACTIONS WITH ACTIVE SUBSTANCES**

Head of the Project: Ph. D. Greta Pifat-Mrzljak

#### **ELECTRON SPIN RESONANCE IN SYSTEMS WITH PARAMAGNETIC PARTICLES**

Head of the Project: Ph. D. Boris Rakvin

#### **MODELLING OF NOVEL CARBON MATERIALS**

Head of the Project: Ph. D. Ante Graovac

#### **INTERACTIONS OF BIOMEMBRANES WITH AMINO ACIDS AND PEPTIDES**



Head of the Project: Ph. D. Vesna Nöthig-Laslo

### **MULTIDISCIPLINARY SEDIMENTOLOGICAL INVESTIGATIONS**

Head of the Project: Ph. D. Halka Bilinski

### **MATTER UNDER EXTREME CONDITIONS**

Head of the Project: Ph. D. Slobodan Bosanac

### **DESCRIPTION AND BEHAVIOR OF QUANTUM SYSTEMS IN INTERACTION**

Head of the Project: Ph. D. Tomislav Živković

## **DEPARTMENT OF ORGANIC CHEMISTRY AND BIOCHEMISTRY**

Ph. D. Vitomir Šunjić, Head of the Division

Programmes (until 30<sup>th</sup> june 2002):

### **SELECTIVE PROCESSES ON MOLECULAR AND SUPRAMOLECULAR LEVEL**

Head of the Programme: Ph. D. Vitomir Šunjić

#### **Research programme:**

Research on the specific fields of organic chemistry and biochemistry has been profiled within this Program, such as combined computational and spectroscopic studies of new molecular structures, in particular those with extended  $\pi$ -electronic systems, primarily by NMR spectroscopy, study of the receptor-selective peptides and glycopeptides, study of the structure and function of hydrolytic enzymes, chemistry of the gelating systems, specifically the group of photoinducible gels, supramolecular chemistry the compounds with specific biological activities (DNA intercalators, molecular receptors with polycyclic units), and with catalytic properties (macrocyclic ligands for catalytic organometallic complexes).

The scientific results are published in 22 original papers, 2 diploma works and 4 dissertations. The members of laboratories which are the part of this Program have had 22 participations at conferences, what included 4 invited lectures, 4 oral presentations and 14 posters.

### **ELECTRONIC STRUCTURE AND DYNAMICS OF ORGANIC MOLECULES**

Head of the Programme: Ph. D. Mirjana Eckert-Maksić

#### **Research programme:**

The final report for research accomplished within the program was sent to Ministry of Science and Technology in 2001. Hence, the results of investigation performed in 2002 are incorporated in the reports of the projects: 0098056 (supervisor: Ph. D. Mirjana Eckert-Maksić), 0098057 (supervisor: dr. sc Goran Baranović), 0098058 (supervisor: Ph. D. Zvonimir Maksić) i 0098059 (supervisor: Ph. D. Dražen Vikić-Topić).

Projects:

### **STEREOSELECTIVE SYNTHESIS AND CATALYSIS**

Head of the Project: Ph. D. Vitomir Šunjić

### **NEW OPTICALLY ACTIVE MATERIALS**

Head of the Project: Ph. D. Vladimir Vinković

## **SYNTHESIS, MOLECULAR STRUCTURE AND FUNCTION OF POLYCYCLIC MOLECULES**

Head of the Project: Ph. D. Kata Majerski

## **SUPRAMOLECULAR ORGANISATION IN GELS, MOLECULAR RECOGNITION AND CATALISYS**

Head of the Project: Ph. D. Mladen Žinić

## **DESIGN AND SYNTHESIS OF BIOACTIVE PEPTIDES, GLYCOPEPTIDES AND BIOMARKERS**

Head of the Project: Ph. D. Štefica Horvat

## **HYDROLASES – FROM ISOLATION TO FUNCTION**

Head of the Project: Ph. D. Marija Abramić

## **REACTIVE INTERMEDIATES IN THE GROUND AND EXCITED STATES**

Head of the Project: Ph. D. Mirjana Eckert-Maksić

## **EXTENDED PI- SYSTEMS AND MOLECULAR SPECTROSCOPIES**

Head of the Project: Ph. D. Goran Baranović

## **PROTON AFFINITIES AND THE PROTON TRANSFER REACTIONS**

Head of the Project: dr.sc. Zvonimir Maksić

## **NUCLEAR MAGNETIC RESONANCE AND CALCULATIONS OF BIOORGANIC MOLECULES**

Head of the Project: Ph. D. Dražen Vikić-Topić

## **POTENTIAL ANTITUMOR DRUGS**

Head of the Project: Ph. D. Štefica Horvat

## **DIVISION OF MATERIALS CHEMISTRY**

Ph. D. Svetozar Musić, Head of the Division

Programme (until 30<sup>th</sup> june 2002):

### **SCIENCE AND TECHNOLOGY OF MATERIALS**

Head of the Programme: Ph. D. Svetozar Musić

#### **Research programme:**

In the frame of realization of the research programme "Science and technology of materials" a significant contributions to the fundamental knowledge in chemistry and physics have been made. A population balance model of crystallization of zeolites from clear aluminosilicate solutions which includes the warming up of the crystallizing system from the ambient temperature to crystallization one, has been developed. The validity of the developed model is evaluated by correlation of calculated kinetics of crystal growth and crystallization with the measured ones, during crystallization of analcime from clear aluminosilicate solution.

Influence of temperature and composition of the reaction mixture on the synthesis of pure, small crystals of zeolite A ( $< 1 \mu\text{m}$ ) from clear aluminosilicate solutions, without the presence of organic templates was investigated. The crystallization field for the

crystallization small crystals of zeolite A ( $< 1 \mu\text{m}$ ) in pure form was defined on the basis of this investigation.

Kinetics of exchange processes between the sodium ions from zeolite A and cadmium, copper and nickel ions from solution containing different contents of sodium ions were studied by measuring the changes in the concentrations of relevant cations in the solid and the liquid phase during the exchange processes. Analysis of the kinetic data showed that a second-order chemical exchange is possible rate-determining step of the exchange process. The equilibrium uptake of the exchangeable cations from the solution decreases with the increasing concentration of sodium ions in the liquid phase in accordance with the mass action law derived from the proposed model of the exchange process.

We recommend the chapters: B. Subotić, Nucleation and Crystal Growth of Zeolite Systems, and Lj. Brečević, Crystall Growth Kinetics and Mechanisms, published in Encyclopaedia of Surface and Colloid Science, A. Hubbard, ed. (Marcel Dekker Inc. 2002), as well as B. Subotić, J. Bronić, Theoretical and Practical Aspects of Zeolite Crystal Growth (Marcel Dekker Inc., in press).

In the past period of time a systematic investigation of spontaneous precipitation of magnesium phosphates has been completed. The effect of different initial conditions, e.g. type of reactants, reactant concentrations and temperature, have been studied. Precipitates were characterized by means of a number of physical chemical methods and techniques. Struvite ( $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ ) was found to be the predominant phase formed in a wide range of reactant concentrations, while newberyite ( $\text{MgHPO}_4 \cdot 3\text{H}_2\text{O}$ ) appears only at  $\text{pH} < 6.5$  and relatively high magnesium concentrations. The thermodynamic solubility products of struvite at two temperatures were calculated, the dissolution kinetics of dendritic and rod-like crystals of struvite in water were determined as well as the activation energies for these processes. Analysis of the kinetic data suggested the diffusion of constituting ions away from the surface of dissolving crystal or the desorption of ions from the crystal adsorption layer, as the possible rate determining mechanisms of struvite dissolution. The study of transformation kinetics of anhydrous calcium sulphate to calcium sulphate dihydrate in aqueous solutions has also been completed. The transformation process was found to be solution-mediated. This was supported by a proper mathematical model, which takes into account the experimentally determined initial solution calcium concentration and mass concentration of the solid phases as well as the rate constants and mechanisms of the processes involved in the transformation: dissolution of anhydrite, dissolution of dihydrate and crystal growth of dihydrate. The values of activation energies obtained, support the assumption that the anhydrite dissolution and the dihydrate growth were controlled by processes at the crystal surface and that the dihydrate dissolution was most probably a diffusion controlled process.

In the frame of the project "Synthesis and microstructure of metal oxides and oxide glasses" the relations between the chemical synthesis of metal oxides and oxide glasses on the one side and the chemical, microstructural and physical properties on the other, were investigated. These investigations were performed using a several model systems. Thermal decomposition of iron choline citrate ( $\text{C}_{33}\text{H}_{57}\text{Fe}_2\text{N}_3\text{O}_{24}$ ) has been investigated using X-ray powder diffraction, FT-IR and  $^{57}\text{Fe}$  Mössbauer spectroscopies. Iron choline citrate was found to be suitable for preparation of nanocrystalline magnetite. Very fine  $\text{SnO}_2$  powders were produced by (a) slow and (b) forced hydrolysis of aqueous  $\text{SnCl}_4$  solutions and (c) hydrolysis of tin(IV)-isopropoxide dissolved in isopropanol (sol-gel route) and then characterized by XRD, FT-IR and laser Raman spectroscopies, TEM and BET. The XRD patterns showed the presence of cassiterite structure. Very fine  $\text{SnO}_2$  powders showed different features in the FT-IR spectra, depending on the route of their synthesis. The additional Raman band at 500, 435 and  $327 \text{ cm}^{-1}$  were recorded for nanosized  $\text{SnO}_2$  particles produced by forced hydrolysis of  $\text{SnCl}_4$  solutions. On the basis of

aggregation differences of nanosized SnO<sub>2</sub> particles the phonon mode at 327 cm<sup>-1</sup> was attributed to the confinement effect of the phonons in the 1D chain. The influence of synthesis procedure on the crystallization and properties of zinc oxide has been also investigated. A new method of the synthesis of nanosized ZnO<sub>2</sub> particles (~ 10 to 20 nm) was found. This new method of the synthesis of metal oxide particles was successfully applied in the synthesis of RuO<sub>2</sub> and acicular α-FeOOH at pH ~ 14. Rhodium has found important applications in the catalytic chemistry. In these applications, rhodium undergoes different oxidation/reduction reactions. In the frame of the present project the formation of rhodium oxides and the corresponding phase transformations were investigated. Noncrystalline metallic rhodium was produced, and the size of nanocrystallites varied between 4 and 7 nm. Various factors that influence the appearance of a tetragonal ZrO<sub>2</sub> polymorph at room temperature have been extensively investigated. Glass-ceramics containing mainly Li<sub>2</sub>Si<sub>2</sub>O<sub>5</sub> and a small amount of Li<sub>3</sub>PO<sub>4</sub> in crystalline phase were studied by integral and by partial thermally stimulated depolarization current (TSDC) in the temperature range, 173 to 373 K.

Physico-chemical effects of ionizing radiations in various model and real systems have been investigated. The investigations of the nature and fate of the reactive short-lived species formed by the radiolysis (electrons, positive ions, excited molecules and free radicals) were also performed. Dosimetry systems based on inducing thermoluminescence of solids or on inducing permanent chemical changes in solutions were investigated. Induction of certain biologically relevant chemical changes in simple model systems and technological applications of irradiation in pharmaceutical and medical materials and foods were also investigated.

Reliable kinetic data on the reaction between Fe(II) ion and t-butoxyl radical, the model reaction for the reactivity of transition metal ions with biological alcoxyl radicals, were obtained by laser flash photolysis. Quantitative data about the complexation of Fe(III) ion in non-aqueous solutions, which is a suitable model for free radical reactions in lipophilic media, were obtained. The experiments with free diffusion of oxygen into samples of unsaturated fatty acids pointed to the importance of availability of oxygen in order to arrive at correct kinetic parameters, such as oxidizability.

The experiences with the use of irradiation for microbial decontamination of botanical materials, of other natural substances which are used in cosmetics, as well as of the successful decontamination by irradiation of some complex final products, were described.

In radiation modification of polymers, the reactions proceed in heterogeneous conditions mainly, and the mechanism of the process can be determined by chemical reactivity and structural and phase transitions of the system in the course of reaction. The goal of our investigation is to determine the role of chemical and structural factors in cross-linking of unsaturated polyester resins as a model system. A combination of different research methods was applied. In our laboratory the method of electrical conductivity and calorimetric method were developed. These methods would help following the course of cross-linking and NIR spectrophotometry was applied in order to investigate the nature of liquid-liquid transition observed in unsaturated polyester resins in investigated temperature range. We expect that our results may essentially contribute to the elucidation of controversy in literature concerning the role of liquid-liquid transitions. It is expected that the possible effect of liquid-liquid transition on cross-linking reaction could be explained. The effects of polymer structure, composition of polymer blends and effect of modification by ionizing radiation on polymer properties, are investigated.

New intermetallic compounds of the general composition RENi<sub>5-x</sub>Ga<sub>x</sub> (RE=rare earth) were prepared and their interaction with hydrogen was studied. It was found that all ternary intermetallic compounds react reversibly with hydrogen, and the hydrogen equilibrium pressure and the amount of absorbed hydrogen decrease with the

increased amount of gallium in the system. Relaxations in  $\text{Li}_2\text{Si}_2\text{O}_5$  were studied by the method of thermally stimulated depolarization current.

The research programme is related to the synthesis and characterization of the new inorganic species comprising hexanuclear halide clusters of niobium, tantalum, molybdenum and tungsten, and the investigation of superconducting oxides. The new compounds are characterized by spectroscopic (IR, UV/VIS) and magnetic measurements, as well as by the use of X-ray diffraction on single crystals and polycrystalline samples. The new cluster compounds of the composition  $[\text{Ta}_6\text{Br}_{12}(\text{H}_2\text{O})_6]\text{X}_2 \cdot \text{trans-}[\text{Ta}_6\text{Br}_{12}(\text{OH})_4(\text{H}_2\text{O})_2] \cdot 18\text{H}_2\text{O}$  ( $\text{X} = \text{Cl}, \text{Br}$ ) have been prepared. The complexes crystallize in the triclinic crystal system, space group  $P\bar{1}$ , and contain two  $[\text{Ta}_6\text{Br}_{12}]^{n+}$  ( $n = 2, 4$ ) units of different oxidation states in the same molecule. The complexes were obtained from aqueous solutions in the presence of copper(II) which catalyzes partial oxidation of  $[\text{Ta}_6\text{Br}_{12}]^{2+}$  to  $[\text{Ta}_6\text{Br}_{12}]^{4+}$ . Mixed-ligand clusters of the  $[(\text{M}_6\text{X}_{12})\text{X}_2(\text{RCN})_4]$  ( $\text{M} = \text{Nb}, \text{Ta}; \text{X} = \text{Cl}, \text{Br}; \text{R} = \text{Et}, n\text{-Pr}, n\text{-Bu}$ ) composition with nitrile molecules along with halogen atoms in terminal octahedral coordination sites of the  $[\text{M}_6\text{X}_{12}]^{2+}$  units, have been prepared. The compounds belong to not numerous class of niobium and tantalum clusters containing N-donor molecules as ligands. With relatively low chemical bond energy of nitrile molecules in terminal octahedral coordination sites of the  $[\text{M}_6\text{X}_{12}\text{L}_6]^{n+}$  units, the new species could be used as precursors for the reactions of these clusters in non-aqueous media with ligands not containing oxygen as donor atoms.

#### Projects:

#### **RESEARCH OF THE CRYSTALLIZATION PROCESS AND USE OF THE ZEOLITES**

Head of the Project: Ph. D. Boris Subotić

#### **PROCESSES AND INTERACTIONS IN HETEROGENEOUS SOLID/LIQUID SYSTEMS**

Head of the Project: Ph. D. Ljerka Brečević

#### **SYNTHESIS AND MICROSTRUKTURE OF METAL OXIDES AND OXIDE GLASSES**

Head of the Project: Ph. D. Svetozar Musić

#### **PHYSICO-CHEMICAL EFFECTS OF IONIZING RADIATIONS**

Head of the Project: Ph. D. Dušan Ražem

#### **SYNTHESIS, CHARACTERISATION AND MODIFICATION OF POLYMERS BY IONISING RADIATION**

Head of the Project: Ph. D. Franjo Ranogajec

#### **INTERMETALLIC COMPOUNDS AND METAL HYDRIDES**

Head of the Project: Ph. D. Želimir Blažina

#### **SUPERCONDUCTING OXIDES AND POLYNUCLEAR METAL COMPLEXES**

Head of the Project: Ph. D. Nevenka Brničević

#### **INFLUENCE OF DOPANDS ON THE STRUCTURE AND PROPERTIES OF MATERIALS FOR TECHNICAL APPLICATIONS**

Head of the Project: Ph. D. Biserka Gržeta

## DEVELOPMENT OF AN ADAPTABLE TECHNOLOGICAL PROCEDURE FOR THE PRODUCTION OF PRECIPITATED CALCIUM CARBONATE

Head of the Project: Ph. D. Damir Kralj

## DEPARTMENT OF MOLECULAR GENETICS

Ph. D. Đurđica Ugarković, Head of the Division

Programme (until 30<sup>th</sup> June 2002):

### THE STRUCTURE, FUNCTION AND EVOLUTION OF THE CELL GENOME

Head of the Programme: Ph. D. Đurđica Ugarković

#### Research programme:

Laboratory of Microbial Genetics has studied the role of the RecBCD enzyme in the processes of DNA metabolism in *Escherichia coli*. RecBCD enzyme participates in homologous genetic recombination, DNA repair, cell viability and degradation of foreign and damaged host DNA. It is well known that the repair of double strand breaks after  $\gamma$ -irradiation in wild type *Escherichia coli* lysogenic for  $\lambda$  *cl857 red3* is more efficient when  $\lambda$  Gam protein is present. Gam dependent radioresistance, a phenomenon discovered in this laboratory, requires the interaction of RecBCD enzyme with the Gam protein of phage  $\lambda$ . The effect of the RecA loading- deficient *recB* (*recB*<sup>D1080A</sup>) mutation on conjugational recombination in the presence of the Gam protein has been studied. The obtained results show that RecA loading activity is not inhibited by the RecBCD-Gam complex.

From the investigation of genes/proteins in marine sponges (Porifera), the most simple extant multicellular animals, studied in the Laboratory for Molecular Genetics, we obtained valuable (bio)information about: (1) the complexity of the genome in the ancestral organism, common to all metazoan animals and (2) the origin and ancestry of certain introns. The findings point to the sponges as an excellent model organism for molecular evolutionary studies. In *Streptomyces rimosus* we discovered: (1) a new type of the promoter, that controls transcription of the *recA* gene and (2) a new type of the lipase. After the search of genomic databases we identified this new promoter in front of many *Streptomyces* genes. Only two lipases of this type are so far reported from the bacteria.

Study of organization and evolution of highly repetitive DNA sequences present in the centromeric and telomeric regions of the chromosomes has been performed in the Laboratory for Molecular Genetics of Eukaryotes. Characterization of satellite DNAs from insect genus *Palorus* revealed their conservation in nucleotide sequence, tandem organization and chromosome localization for long evolutionary periods. Conservation of the satellites through evolutionary period of around 70 million years indicates their potential functional significance. Model of satellite DNA evolution based on "library" concept was presented and discussed in the review article. In collaboration with Institute for Molecular Biology in Barcelona telomeric and subtelomeric sequences have been characterized in marine molluscs and echinoderms. It has been shown that telomeric motif characteristic for this group of invertebrate species is identical to those specific for vertebrates and probably represents an ancient telomeric sequence.

Gene Regulation Laboratory is broadly concerned with the regulation of gene expression in eukaryotes. The process of gene transcription in higher eukaryotes is a complex process involving a variety of protein factors in addition to RNA polymerase II, the enzyme responsible for transcribing protein coding genes. Our research currently centres on questions regarding the fundamental mechanisms of gene

transcription in eukaryotic cells where we use the yeast *Saccharomyces cerevisiae* as a model system. One aspect of our work centres on the function and regulation of the general initiation factor TFIIF. This factor is essential to the initiation and elongation phases of transcription by RNA polymerase II. Since transcriptional elongation is the major mechanistic target of the HIV Tat regulatory gene, insights into the role of TFIIF in transcriptional regulation will aid in our understanding of the mechanisms by which viruses usurp the cellular machinery. Another research theme is the intra-cellular signalling pathway which connects mitochondrial function to nuclear gene expression. Lastly, we have begun to study human transcription factors in a heterologous yeast system. The aim is to develop assays for disease related transcription factors in yeast which will aid in generating high-throughput systems for drug development.

Broad interest of Laboratory for Experimental Cancerology is to investigate role of telomeres in carcinogenesis and cell aging. Telomeres are involved in basic cell functions, such as cell division, cell aging or maintenance of immortal state of tumor cells and unicellular eukaryotes. We presented experimental evidence demonstrating that inhibition of the onset of Sudden Senescence Syndrome (SSS) by viral protein SV40 Tg, greatly reduces the appearance of senescent cells in the culture and results in an increase in the population doublings (PD) to that of the number of cell generations (CGs). This is what causes the observed lifespan extension. Our results also provide an explanation for "additional" telomere shortening during this "extended" lifespan. The results indicate SSS as the single, primary mechanism of cell senescence. We also investigated the ability of human immunodeficiency virus-1 (HIV-1) tat/nef-defective genomes containing diphtheria toxin A chain gene (DTA) to inhibit replication of HIV in human cells. Each of the DTA-containing plasmids strongly suppressed HIV production, whereas the defective non-DTA containing plasmids did not interfere with the virus growth. This may be taken into consideration as a therapy approach to treatment of HIV infection, based on its selective and specific toxicity only to HIV infected CD4- positive cells.

Cell response to physical, chemical and biological agents is studied in the Laboratory for Genotoxic Agents. This is highly complex process that depends on the type of the damaging agent as well as on the cell status. The network of proliferation, survival and apoptotic genes will determine the fate of damaged cells. In infection with adenoviruses, fiber protein plays important role. Our main results obtained in the last year are: a) the activation of MAP kinases is important in response of tumor cells to cisplatin, and probably in resistance to this drug; b) specific compounds targeted to glutathione may reduce the growth of tumor cells, c) the shortening of adenovirus fiber length slightly influences its binding, but is not followed by successful entry. In the Laboratory for Neurochemistry and Molecular Neurobiology further neurochemical, molecular-genetic and behavioral characterization of their original experimental model of animals with altered serotonin homeostasis—"Wistar-Zagreb 5HT rat" was performed. Also, neurochemical and molecular genetic studies of serotonergic parameters in healthy population and neuropsychiatric patients were done. Former studies on hydrodynamics of the cerebrospinal fluid (CSF) are continued focusing on the validation the model of perfusion of the CSF system using indicator substance, a method for calculation of the CSF formation, and on development of a new model of measuring the CSF formation.

Laboratory for Electron Microscopy focuses on structure and function of plastids and cytoskeleton. Combination of genetic and imaging approaches resulted in important insights into several aspects of the structure and the dynamics of the actin cytoskeleton in the model organism *Dictyostelium*. In collaboration with W. Baumester's group at the Max-Planck-Institut für Biochemie in Martinsried, cryoelectron tomography was successfully applied to image molecular complexes and ultrastructure of the actin cytoskeleton in intact *Dictyostelium* cells. For the first time, macromolecular architecture of an unperturbed environment inside eukaryotic

cells was visualized at a resolution of 5 to 6 nanometers. In a search of novel components involved in chloroplast division and biogenesis, a new *Arabidopsis* protein with a unique molecular structure was discovered. The protein, called ARTEMIS for *Arabidopsis thaliana* envelope membrane integrase, has a carboxy-terminal domain that shows sequence similarity to YidC, Oxa1 and Alb3 proteins. These proteins are important for integration of membrane proteins involved, respectively, in protein secretion in bacteria, protein import to the mitochondrion in budding yeast, and assembly of the photosynthetic apparatus in plants. In the Laboratory for Chemical Biology research on the structural basis of physiological activity was focused on plant hormones. A number of other biomolecules were studied by spectroscopic methods (in particular, Nuclear Magnetic Resonance).

In Laboratory for Biocenology the field studies of marine algae and coastal halophytes along Croatian mainland shores and Adriatic islands were done. A detailed ecological map of vegetation habitats across Croatia is mostly completed in GIS electronic form. By the intense studies of fungi across Croatia, 78 taxa new to Croatian mycoflora were registered.

#### Projects:

#### **THE ROLE OF RECOMBINATION IN DNA REPAIR AND GENOME STABILITY**

Head of the Project: Ph. D. Erika Salaj-Šmic

#### **REGULATION OF RECOMBINATION AND RECOMBINATIONAL REPAIR**

Head of the Project: Ph. D. Mirjana Petranović

#### **GENES AND GENOMES OF EVOLUTIONARY CONSERVED AND ECONOMICALLY IMPORTANT SPECIES**

Head of the Project: Ph. D. Vera Gamulin

#### **STRUCTURE AND FUNCTION OF PLASTIDS AND CYTOSKELETON**

Head of the Project: Ph. D. Nikola Ljubešić

#### **EVOLUTIONARY DYNAMICS OF SATELLITE DNAs**

Head of the Project: Ph. D. Đurđica Ugarković

#### **ORGANIZATION OF HETEROCHROMATIC DNA SEQUENCES IN INVERTEBRATES**

Head of the Project: Ph. D. Miroslav Plohl

#### **CELL RESPONSE TO PHYSICAL, CHEMICAL AND BIOLOGICAL NOXA**

Head of the Project: Ph. D. Maja Osmak

#### **TRANSCRIPTIONAL REGULATION IN EUKARYOTES**

Head of the Project: Ph. D. Mary Sopta

#### **MOLECULAR MECHANISMS OF IMMORTALIZATION AND CELLULAR AGING**

Head of the Project: Ph. D. Ivica Rubelj

#### **STRUCTURE, FUNCTION AND REGULATION OF PLASMINOGEN SERINE PROTEASES**

Head of the Project: Ph. D. Branko Brdar

#### **DYNAMICS AND GENETICS OF BIOACTIVE MOLECULES**

Head of the Project: Ph. D. Volker Magnus



## **MOLECULAR PATHOPHYSIOLOGY OF SEROTONERGIC TRANSMISSION**

Head of the Project: Ph. D. Branimir Jernej

## **HYDRODYNAMICS OF THE CEREBROSPINAL FLUID**

Head of the Project: Ph. D. Darko Orešković

## **ENDEMIC AND RELICT PHYTOCENOSSES IN CROATIA AND THEIR MYCOFLORA**

Head of the Project: Ph. D. Andrija-Željko Lovrić

## **DIVISION OF MOLECULAR MEDICINE**

Prof. Ph. D. Krešimir Pavelić, Head of the Division

Programme (until 30<sup>th</sup> June 2002):

### **CANCER RESEARCH**

Head of the Programme: Ph. D. Krešimir Pavelić

#### **Research programme:**

The "Cancer Research" program covered basic and applied research into the molecular-genetic and cellular basis of cancer. The program also covered research into the molecular genetics of diseases caused by so-called dynamic mutations, namely the accumulation of repeated trinucleotide sequences.

The results of the research were published in 2002 in 33 of scientific journals indexed in the Current Contents. In the first section, we shall mention some of the results which were comprehensively described within the framework of individual projects. We shall also address the application of the results of these researches, since this aspect is not mentioned in the results of the reports presented in this document.

A significant part of the results found their direct or potential application within the framework of molecular-genetic diagnostic procedures, newly discovered genes as potential genetic markers, new procedures in treating patients with malignant tumors and new procedures in the domain of tissue engineering. Here are some examples. On the basis of the program, the following genetic methods were developed and included into routine clinical practice: determining the genetic predisposition to develop medullary cancer of the thyroid gland within the MEN-2 syndrome (analysis of the *RET* gene), the diagnostics of the familial adenomatous polyposis (analysis of the *APC* gene), determining the tendency to develop nonpolyposis colon cancer (the genes of the group responsible for HNPCC), diagnostics of Duchenne's muscular dystrophy, Huntington's disease, fragile X syndrome, cystic fibrosis, Gorlin's syndrome, familial melanoma, genotyping of the human papilloma viruses, presence of cytomegalovirus, adeno-associated virus, *Helicobacter pylori*, *Eikenella corrodens*, *Actinobacillus actinomycetemcomitans*, *Porphyromonas gingivalis*, *Bacterioides forsythus*, *Leptotrichia buccalis*, *Streptococcus mitis*, *Fusobacterium nucleatum* and *Prevotella intermedia*.

Within the program, a new system for detecting a mutation launched by the Swiss company Elchrom Scientific (Spreadex<sup>TM</sup> and GMA<sup>TM</sup> gels SEA<sup>®</sup> 2000 Apparatus) was tested. The testing resulted in a very successful application of the system for detecting mutation of the cystic fibrosis gene ( $\Delta F508$  and  $\Delta I507$ ) and the *APC* gene (familial adenomatous polyposis of the colon), which was published in the company's promotional material.

A new method for the quick differential diagnosis of diseases caused by dynamic mutations was also discovered. The expand long PCR method for diagnosing the

fragile X syndrome is routinely applied. The application of this method in diagnosing other disease caused by dynamic mutations is also being tested. The method was first described by the researchers involved in this program and is today routinely applied.

Two new genes were discovered – one in human subjects, the other in mice. The *USP25* gene, originating from human subject, is located on chromosome 21. A gene participating in the development of the T-cells in mice was also discovered; cDNA for the U2 snRNP-A protein like *USP25* was entered into the GENE BANK. The role of the two newly discovered genes is being researched in other laboratories.

The research into hyperthermia in treating tumor patients is being applied. The results of our research into cisplatin and etoposides were included in some clinical protocols. The results of the testing of some new potential medications have entered Phase I or Phase II of clinical trials.

The results of the work in the field of genetic treatment are being partially applied. The gene therapy model using the suicide gene (HSVtk) is in clinical application in treating head and neck malignant tumors. Other genetic approaches based on the application of the tumor suppressor genes *p53*, *p21*, *nm23-H1/H2* and *p73* are either completed or are being researched on *in vitro* or *in vivo* models.

The results obtained through antisense treatment for genes of the IGF family could also soon be clinically applied. Some of the results are used at the Dermato-Venerological Clinic of the Medveščak Health Center in Zagreb. The GaAs laser is successfully used in patients with ulcer cruris. Furthermore, findings on photodynamic treatment have served as the basis for clinical application which is about to be implemented.

The results of the research into mechanisms of action for Met-Enkephalin (MENK) allow for planning MENK in treatment. Mono- and polyvalent vaccines, containing viral subunits and prepared as a water/oil/water emulsion were tested on 19,000 farm-grown and fattened chickens and demonstrated a remarkable protective efficiency in application. The possibility of using the synthetic peptide Met-Enkephalin (peptide M) as an immunomodulator in autoimmune diseases and the benefit from using the methods of machine learning in evaluating the impact of proteins on the survival of carcinoma patients, on the development of diabetic retinopathy and on the development of kidney stones were confirmed.

In the program of tumor gene therapy, we completed our research into the suicide gene approach. The suicide gene we used was the Herpes simplex virus thymidine kinase gene (HSVtk), which, when incorporated into tumor cells, rendered the infected cell sensitive to the otherwise nontoxic drug ganciclovir (GCV). The antitumor suicide gene approach was fully effective in both *in vitro* and *in vivo* models. In the course of 2002, we proceeded with exploring the therapeutic suppressor genes *p53* and *p21* in tumor gene therapy. We confirmed our hypothesis that the programmed cell death (apoptosis) counterparts in the mechanisms of tumor growth inhibition. The exogenous *p53* gene caused apoptosis in tumor cell lines that had a mutated or inactivated endogenous *p53* gene, while the apoptosis induced by *p21* gene overexpression was seen only after a prolonged period of incubation with the virus-carrying *p21* transgene. Both genes were equally effective in inducing apoptosis in mouse carcinoma cell line. The main question concerning the *in vivo* therapeutic approach with *p53* and *p21* genes is whether the ectopic expression of therapeutic genes can stop or diminish *in vivo* tumor growth, and we started experiments to resolve this question. We also started experiments on evaluating the antitumor activity of the *p73* gene. We found that the human *p73* gene generates an NH<sub>2</sub>-terminally truncated isoform that is frequently overexpressed in a variety of human cancers but not in normal tissue. We are proceeding with research into the role of the mutated *p73* protein in initiating or keeping a transformed phenotype in order to find a way of interfering with malignant transformation by the use of gene therapy.

Hereditary syndromes have facilitated understanding of the molecular mechanisms that may cause carcinogenesis and malformations during development. *PTCH*, the gene responsible for Gorlin syndrome, is a tumor suppressor involved in the genesis of various malformations and tumors that appear with greater incidence in the syndrome than in the general population. It has recently been found that *PTCH* functions within the newly discovered SHH/*PTCH*/*SMO* signaling pathway. Our research has proved by indirect methods (analysis of heterozygosity and SSCP) that the incidence of *PTCH* mutations in sporadic tumors and malformations is much greater than that of the syndrome itself. SSCP analysis established the patterns of the most frequent *PTCH* gene polymorphisms. Our first results from analyzing gene expression in the SHH/*PTCH*/*SMO* pathway indicate aberrant behavior of the *SMO* gene and the target gene *GLI*, supporting the hypothesis that all the pathway genes should be considered.

In order to select the immunologically active proteins, polypeptides and peptides for the design of vaccines that generate anti-viral immunity and a specific response against antigens associated with tumors and immune-mediated diseases, a complementary protein recognition model was proposed and experimentally tested. The vaccine preparation and administration were studied in order to find the optimal efficacy of the protein and peptide vaccines. Newly-introduced molecular biology methods for the identification of poultry viruses will enable the design and preparation of the appropriate vaccines for effective immunoprotection.

We also studied the mechanisms and factors involved in lymphocyte differentiation and the genes orchestrating this process. These mechanisms are strictly controlled. One of the lymphocyte development control systems is the activation of certain transcription factors that define the place, time and speed of target gene expression. The most important transcription factors in lymphocyte development are proteins from the *Ikaros* gene family (*Ikaros*, *Aiolos*, *Helios*). We found a very high homology between the mouse and the human *Aiolos* gene. In human material, we detected several *Aiolos* isoforms that are the result of alternative mRNA splicing. Given the predicted importance of these transcriptional factors in lymphocyte maturation, we investigated *Helios* mRNA expression in human lymphocytes in order to find out its possible role in human lymphoproliferative disorders.

The myelodysplastic syndrome (MDS) comprises a heterogeneous group of clonal bone marrow disorders characterised by abnormal differentiation and maturation of myeloid cells, bone marrow failure and a genetic instability with enhanced risk of transforming into secondary leukemia. As ACE has been shown to enhance the recruitment of bone marrow stem cells into the S-phase of the cell-cycle, we chose to investigate its role in dysfunctional hemopoiesis of the MDS. Multiparametric analysis of biochemical parameters to ACE expression and ACE genotype showed a statistically significant negative correlation between ACE expression and the number of platelets. Polymorphism of the ACE gene had no significant influence on the survival of MDS patients.

A major research topic is the evaluation of oxidative stress under experimental conditions in vitro and in vivo that resemble clinical disorders based on oxidative stress. We primarily studied the effects of 4-hydroxynonenal (HNE), the end-product of lipid peroxidation, on the proliferation and differentiation of normal and malignant cells and their gene expression. The results indicated that HNE has a complex role in the processes of cell proliferation and differentiation and tumorigenesis; however, additional studies are needed to further clarify the role of HNE in cell growth control. We concluded our molecular genetic studies of hereditary diseases concerning fragile chromosome X syndrome and Huntington disease. The molecular and clinical data show that FRAXE mental retardation is phenotypically very mild and that every woman with a mentally retarded and/or learning disabled family member should be investigated for the FRAXA and FRAXE loci of the fragile X syndrome.

Projects:

**TRANSCRIPTIONAL CONTROL OF LYMPHOCYTE DEVELOPMENT – ITS ROLE IN LEUKEMOGENESIS**

Head of the Project: Ph. D. Mariastefania Antica

**REGULATION OF ECTOPEPTIDASES AND OPIOID RECEPTORS EXPRESSION**

Head of the Project: Ph. D. Jelka Gabrilovac

**MOLECULAR MECHANISMS IN THE PATHOGENESIS OF NEUROENDOCRINE TUMORS**

Head of the Project: Ph. D. Koraljka Gall-Trošelj

**GENETIC AND MOLECULAR PROGNOSTIC FACTORS OF CERVICAL CANCEROGENESIS**

Head of the Project: Ph. D. Magdalena Grce

**EMBRYONIC CELL PRODUCTION OF PANCREATIC-LIKE ISLETS**

Head of the Project: Ph. D. Mirko Hadžija

**VIRUS ANTITUMOROUS ACTION AND ONCOLYTIC VIRUS VACCINE**

Head of the Project: Ph. D. Mislav Jurin

**MOLECULAR GENETICS OF GASTROINTESTINAL TUMORS**

Head of the Project: Ph. D. Sanja Kapitanović

**ROLE OF FHIT GENE IN NEUROENDOCRINE TUMORS**

Head of the Project: Ph. D. Šimun Križanac

**THE SHH/PTCH/SMO SIGNALING PATHWAY IN CANCER AND DEVELOPMENT**

Head of the Project: Ph. D. Sonja Levanat

**OXIDATIVE/ANTIOXIDATIVE STATUS AFTER TREATMENT WITH OPIOIDS/OPIATES**

Head of the Project: Ph. D. Tanja Marotti

**NEUROPHARMACOLOGY OF SEROTONERGIC SYSTEM**

Head of the Project: Ph. D. Dorotea Muck-Šeler

**MOLECULAR MECHANISMS OF IMMUNOSUPPRESSION**

Head of the Project: Ph. D. Renata Novak Kujundžić

**TUMOR GENE THERAPY – CORRECTION OF ONCOSUPPRESSOR GENES**

Head of the Project: Ph. D. Jasminka Pavelić

**GENE OR PROTEIN TRANSDUCTION AND SIGNALLING PATHWAYS IN TRANSFORMED CELLS**

Head of the Project: Ph. D. Krešimir Pavelić

**INSULIN LIKE GROWTH FACTOR FAMILY OF GENES IN LUG CANCER**

Head of the Project: Ph. D. Ljubomir Pavelić

**NEUROTRANSMITTERS IN STRESS AND REGULATION OF GABA<sub>A</sub> RECEPTORS IN VITRO**

Head of the Project: Ph. D. Danka Peričić

### **MODULATION OF IMMUNOLOGICAL RESPONSE BY BIOACTIVE PEPTIDES**

Head of the Project: Ph. D. Biserka Pokrić

### **CYCLOOXYGENASE-2: NEW TARGET FOR CHEMOPREVENTION AND TREATMENT OF COLON TUMORS**

Head of the Project: Ph. D. Radan Spaventi

### **NEW THERAPEUTIC POSSIBILITIES IN BREAST CANCER**

Head of the Project: Ph. D. Josip Unušić

### **ASSESSING FUNCTIONS OF THE HEAT REPEAT IN HUNTINGTIN PROTEIN**

Head of the Project: Ph. D. Oliver Vugrek

### **OXIDATIVE STRESS AND MALIGNANT DISEASES**

Head of the Project: Ph. D. Neven Žarković

### **ORGANOTYPIC SKIN CULTURE IN VITRO**

Head of the Project: Ph. D. Milivoj Boranić

## **CENTER FOR MARINE RESEARCH**

*Ph. D. Nenad Smolaka, Head of the Division*

Programme (until 30<sup>th</sup> june 2002):

### **RESEARCH OF PROCESSES AND ECOLOGICAL RELATIONSHIPS IN THE ADRIATIC**

Head of the Programme: Ph. D. Renato Batel

#### **Research programme:**

The general scope of the program is a better knowledge of the Adriatic Sea taking into account the economical demands of the Republic of Croatia and environmental protection. A prerequisite for the determination of the state and trends in changes conditioned by natural and anthropogenic factors is the knowledge of basic interrelationships and processes in ecosystems and marine organisms. Therefore, complex field and laboratory researches are planned focussed on the: a) determination of physical, chemical and biological characteristics of the Adriatic Sea and its particular areas; b) fundamental study and monitoring of the pelagic ecosystem dynamics, particularly in the northern Adriatic; c) basic studies of benthic ecosystems and biodiversity determination; d) interdependence of pelagic and benthic ecosystems with special regard to "sea blooming"; e) study of pollutants and activity mechanisms at DNA, enzyme and other biochemical characteristics organism levels; f) biochemical and physiological research of marine organisms and development of methods for the determination of toxicological stress; g) study of osmolyte and toxic metals transport in marine organisms; h) efforts in an acceptable management and protection of Adriatic selected areas and organisms; i) education in marine sciences.

Projects:

## **MECHANISM OF LONG-TERM CHANGES IN THE ADRIATIC SEA ECOSYSTEM**

Head of the Project: Ph. D. Danilo Degobbis

## **PROGRAMMED BIOSYNTHESIS AND GENOTOXIC RISK ASSESSMENTS**

Head of the Project: Ph. D. Renato Batel

## **FIZIOLOŠKI I BIOKEMIJSKI INDIKATORI TOKSIKOLOŠKOG STRESA U MORSKIH ORGANIZAMA**

Head of the Project: Ph. D. Bartolo Ozretić

## **ECOPHYSIOLOGICAL STUDIES AND STRESS RESPONSE IN MARINE ORGANISMS**

Head of the Project: Ph. D. Čedomil Lucu

## **CENTER FOR MARINE AND ENVIRONMENTAL RESEARCH**

Ph. D. Božena Čosović, Head of the Division

Programme (until 30<sup>th</sup> june 2002):

### **ENVIRONMENTAL RISK STUDIES IN THE ADRIATIC AND CONTINENTAL REGIONS OF CROATIA**

Head of the Programme: Ph. D. Božena Čosović

#### **Research programme:**

The long term research programme of the Centre for marine and environmental research is focused on the investigation of the biogeochemical cycles of inorganic and organic constituents and natural characteristics of the Adriatic Sea and freshwater systems in Croatia, evaluation of the anthropogenic influence by modelling distribution and behaviour of substances and their speciation in water and at natural phase boundaries and assessment of the impact of inorganic and organic pollution on biological species and communities (ecological risk assessment) using methodology of exposure biomarkers and effect biomarkers and monitoring health condition of aquatic organisms.

These investigations are aimed to give new scientific knowledge for environmental management, water quality management and water use in Croatia. To achieve this goal model laboratory experiments are used together with field observations that are performed in the Adriatic Sea and adjacent estuaries and in the continental surface and groundwaters of the Sava and Danube river basins. Multidisciplinary and interdisciplinary approaches are developed with special attention to education of young scientists in the field of natural sciences, particularly in Oceanography.

Projects:

### **TIDAL AND LONGER-PERIOD DYNAMICS OF THE NORTHERN ADRIATIC**

Head of the Project: Ph. D. Milivoj Kuzmić

### **ANALYSIS AND BIOGEOCHEMISTRY OF ORGANIC COMPOUNDS IN THE AQUATIC ENVIRONMENT**

Head of the Project: Ph. D. Marijan Ahel

### **PHYSICAL CHEMISTRY AND BIOGEOCHEMISTRY OF TRACE METALS IN AQUATIC SYSTEMS**

Head of the Project: dr.sc. Marko Branica

**NATURE AND REACTIVITY OF ORGANIC SUBSTANCES IN MARINE AND ENVIRONMENT**

Head of the Project: Ph. D. Božena Ćosović

**ELECTROANALYTICAL RESEARCH IN LIQUID AND SOLID ELECTROLYTES**

Head of the Project: dr.sc. Milivoj Lovrić

**MODELS AND INFO. SYSTEMS FOR ENVIRONMENTAL PROTECTION AND NAVIGATION MANAGEMENT**

Head of the Project: Ph. D. Ivica Ružić

**PROTECTION OF BIOCOENOTIC BALANCE IN AQUACULTURE RECEIVING WATERS**

Head of the Project: Ph. D. Emin Teskeredžić

**PREPARATION AND PROPERTIES OF METAL SURFACES IN THE ENVIRONMENTAL PROTECTION**

Head of the Project: Ph. D. Marijan Vuković

**INTERFACIAL PROCESSES AND EUTROPHICATION**

Head of the Project: Ph. D. Vera Žutić

**RADIONUCLIDES IN ENVIRONMENTAL SYSTEMS**

Head of the Project: Ph. D. Delko Barišić

**METALS AND CELLULAR BIOMARKERS**

Head of the Project: Ph. D. Biserka Raspor

**PERSISTENT ORGANOHALOGEN POLLUTANTS IN SOME COASTAL AREA OF DALMATIA**

Head of the Project: Ph. D. Mladen Picer

**GEOCHEMISTRY OF RECENT AND ANCIENT SEDIMENTARY SYSTEMS OF THE ADRIATIC PLATFORM**

Head of the Project: Ph. D. Goran Kniewald

**MODELS OF AQUATIC ECOSYSTEMS**

Head of the Project: Ph. D. Tarzan Legović

**MICROBIAL COMMUNITIES AS CATALYSTS IN BIOTRANSFORMATION PROCESSES**

Head of the Project: Ph. D. Dubravka Hršak

**MULTIXENOBIOTIC RESISTANCE MECHANISM AS A BIOMARKER OF ENVIRONMENTAL QUALITY**

Head of the Project: Ph. D. Tvrtko Smital

**DEVELOPMENT OF NEW TYPE OF ELECTROCHEMICAL SENSOR AND MEASUREMENT SYSTEM FOR REACTIVE MICROPARTICLES**

Head of the Project: Ph. D. Vera Žutić

**CONCEPTUAL MODEL FOR BIOLOGICAL TREATMENT OF EFFLUENTS FROM ATRAZINE PRODUCTION**

Head of the Project: Ph. D. Dubravka Hršak

## **DIVISION OF LASER AND ATOMIC RESEARCH AND DEVELOPMENT**

Ph. D. Hrvoje Zorc, Head of the Division

Programme (until 30<sup>th</sup> june 2002):

### **OPTRONIC INSTRUMENTATION OF DEFENSE SYSTEMS**

Head of the Programme: Ph. D. Antun Peršin

#### **Research programme and results:**

1. Imaging optics: In the frames of research of the optical phenomena we made a progress in theory of aberrations of diffraction field. By recognizing that Fresnel diffraction patterns are merely defocused Fraunhofer diffraction patterns, we show that the Fraunhofer criterion can be written precisely in terms of an allowable tolerance on defocus. This new criterion provides insight that is useful to optical designers and engineers who routinely deal with such tolerances distance until to far-field region (where the Fraunhofer diffraction is defined) can be determined based on the defocus tolerances for some application.
2. Non-imaging optics: In 2002 we made a breakthrough with the development of sources for photodynamic tumor therapy. The new source, based on the high density LED array with the peak radiation wavelength at 635 nm, is very good for use in photodynamic therapy with hematoporphyrine and perfect for use with 5-ALA.
3. Optics of thin films: The work on the reverse engineering of the optical thin films has been continued to make a successful refractive index profile. Several oxide materials have been studied and it has been found that each of them has a specific refractive index profile, depending on the intrinsic material properties and deposition conditions respectively.

Projects:

### **PHOTONIC OF IMAGING AND NON IMAGING OPTICAL SYSTEMS**

Head of the Project: Ph. D. Antun Peršin

### **SPECTRAL SOURCES FOR MEDICAL APPLICATION**

Head of the Project: Ph. D. Antun Peršin

## **CENTER FOR NUCLEAR MAGNETIC RESONANCE**

Head of the Center: Ph. D. Dražen Vikić-Topić

#### **Research programme and results:**

Center for NMR spectroscopy at Ruđer Bošković Institute (RBI) is the only academic NMR facility in Croatia. Therefore, even few hundreds of Croatian scientists and researchers from RBI and Universities of Zagreb, Rijeka, Split and Osijek and other governmental institutions use permanently or temporarily the equipment of NMR center. Three NMR spectrometers are in use:

- Varian Gemini 300 MHz (from 1990)
- Bruker Avance 300 MHz (from 2002)
- Bruker Avance 600 MHz (from 2002)



NMR center also possesses SUN Sparc 4 station and different devices for plotting, printing and retrieving of NMR data. Different kinds of measurements of  $^1\text{H}$  and  $^{13}\text{C}$  one- and twodimensional NMR (COSY, NOESY, ROESY, HMBC, HSQC) are performing as well as measurements of other nuclei such as:  $^2\text{H}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{32}\text{P}$ ,  $^{113}\text{Cd}$ ,  $^{199}\text{Hg}$ . From time to time the quantitative NOE measurements and differential NOE measurements are also performing.

NMR investigations performed in Center covered organic, bioorganic and pharmaceutical chemistry. In addition inorganic, physical and analytical chemistry as well as biochemistry researches are carried out. Basic investigations are conducted on natural compounds, sugars, nucleosides and small peptides. Researches in supramolecular chemistry, metal complexation and isotope effects by NMR spectroscopy are also going on. The members of NMR center participate in Ministry of Science and Technology project No. 0098059 "Nuclear Magnetic Resonance Resonance and Calculations of Bioorganic Molecules" under the conduct of D. Vikić-Topić. The NMR investigation of the structure, dynamics and interactions of small biomolecules (peptides, quinolones, etc.) and quantum chemical calculations has been performed. The conformations important for bioactivity are analyzed by NOE measurements, isotope labelling and complexation. Relatively small number of atoms in these molecules enable the precise quantum chemical calculations of their structure, conformation as well as their properties. Calculated NMR parameters (chemical shifts, spin-spin couplings) are correlated with the experimental NMR data for obtaining deeper insight into the structure and nature of interactions in solution. The investigations are supported by other spectroscopy measurements (IR, UV/VIS, Mass spectrometry and X-ray analysis). The knowledge of the structure, conformation and properties of bioorganic molecules is helpful in studying bioprocesses: protein folding, isomerization, ligand-receptor interactions (intrinsic, extrinsic), hydrogen bonding as well as in pharmacokinetics and drug design. Short peptide fragments, 5 to 13 amino acids, can mimic activity of the whole peptide and sometimes they can be even more bioactive than the whole molecule. Such peptide fragments, which repeat many times in molecule, can be used themselves as a drug or can be the lead compounds for the development of classical drugs. Theoretical calculations of nuclear shielding are also performing. In addition applicative investigations with NMR spectroscopy for pharmaceutical and petrochemical industry are carried out as well. The staff of NMR center participate in undergraduate and graduate studies at Faculty of Science, Faculty of Pharmacy and Biochemistry, School of Health Studies, Faculty of Chemical Engineering and Technology and Faculty of Food Technology and Biochemistry of the University of Zagreb, Split and Osijek. NMR center has published few scriptae on NMR spectroscopy for undergraduate and graduate studies. In addition to lectures and practical demonstrations in NMR spectroscopy diploma work, master of science and Ph. D. thesis are completed in NMR center as well.

## LIBRARY

Head of the Library: M. Sc. Jadranka Stojanovski

### Programme and results:

Throughout the year 2002 the Library continued to lead and coordinate the following projects:

*Croatian Science Information System – thematic subsystem Natural Science*  
(<http://prirodo.irb.hr>)

In 2002 the project Natural Science included 26 natural science libraries. Work was conducted on unifying the online catalogue, on co-ordinated acquisition of library material, stimulating the computerisation of libraries, educating the librarians etc.

Productive cooperation with Biomedicine, Engineering and Humanities subsystems has continued. Social Sciences subsystem was also initiated in 2002. Croatian Science Information System, which was initially launched in 1995 by RBI and ten other libraries, is today coordinating over 100 research libraries.

*Online Database Centre* (<http://baze.irb.hr>)

The project to provide the Croatian scientific community with access to commercial and other databases was continued successfully. At this moment the Centre offers its users ten databases: Current Contents, Medline, INSPEC, PsycInfo, Ovid Core Biomedical Collection, Evidence Based Medicine Review, ERIC, WoS, INIS and Ei Village (Compendex). Those are the most significant databases in the fields of biomedicine, physics and engineering. About 4200 registered users research them.

*Croatian Scientific Bibliography CROSBIB* (<http://bib.irb.hr>)

CROSBIB was initially established as a supporting tool for the Ministry of Science and Technology in gathering data about published papers, as a result of activities on various projects. It developed into a comprehensive electronic bibliography, whose major advantages are recentness and completeness of data. The database includes data from 1996 up to the present day, which add up to more than 60000 documents.

*Who is Who in Croatian Science* (<http://tkojetko.irb.hr>)

The objective of the project is to gather in one place data on Croatian scientists. It is possible to search and retrieve the database. The main idea is to promote Croatian scientists at home and abroad, to connect the scientists and to advance communication. At the moment the project is under testing.

*EJOL Electronic Journals online Library* (<http://ejol.irb.hr>)

The main goal of this project is to develop a unique Web interface that provides access to numerous scientific electronic journals, and to the preprint archives, as well as to Croatian media. Particular care has been taken of domestic scientific journals, which are mainly unknown to the international scientific community and cannot be found in other similar databases. The idea of the implementation of the base is to enable registered libraries in Croatia to access the database, by way of electronic access interface, and at the same time to enable libraries to maintain their own electronic and printed subscriptions. EJOL will be accessible to all members of Croatian scientific community, as well as to general public.

In the course of the last year we have undertaken two major parallel projects in the Library:

1. SEND – Electronic Documents Acquiring System (<http://library.irb.hr/send>). To help our customers to get printed and electronic documents not available at our Library, we have developed a web interface, which makes it possible for authorised users to loan documents from Croatian libraries or abroad. The SEND interface started at the end of December 2002 and the first reactions were very favourable. The Library is delivering documents to library users at a favourable rate. Interlibrary cooperation with TIBORDER service (Universitätsbibliothek und Technische Informationsbibliothek Hannover) begun in 2001, because they offered most acceptable terms. Digital documents are delivered via e-mail in 5 days, or books are lent.
2. New online interface for catalogue search, which works faster and better than the “old” one. A recently conducted detailed statistics on access gave us an average result of 130 catalogue searches per day. It could be found at <http://prirodo.irb.hr/katalozi/stats/>

In 2002, the Library acquired 494 books: 389 of which were purchased and 54 were donated to the Library. Seven titles were donated by the SABRE foundation. Forty-four books from Chromos collection were catalogued. The Library has participated in donating books to prisoners: it has collected 159 books.

The Library's collection amounts to 32417 volumes (16000 electronically catalogued so far)

In the year 2002 the Library was subscribed to 383 scientific journals. The subscription to 65 titles (and 11 electronic versions) was covered by the Institute funds, while 249 titles were subsidized by the Ministry of Science and Technology of the Republic of Croatia. The total number of available journal volumes is nearly 27.000. The difficulties caused by frequent delays of incoming copies of periodicals were substantially remedied by the use of electronic journals. The Library's long lasting endeavour to ensure its users access to electronic versions of the journals was in a great deal made possible by contracts between the Ministry of Science and Technology and four major publishers: Elsevier, Wiley, Springer Verlag and Kluwer Academic Publishers. This arrangement made all their e-journals to which various Croatian libraries are subscribed to available, as well as many journals, which are not subscribed to in printed form. Through *ScienceDirect (Elsevier)* 1208 journals are available, from *SpringerLink* 420, by *WileyInterscience* 100, and through Kluwer 757 titles. In total, 2500 subscribed e-publications were at the disposal to the staff of the Ruđer Bošković Institute in 2002!

Apart from such a great number of subscribed e-journals, the choice was further extended by trial access, for instance, to *BlackwellSynergy* (407 titles), *Institute Of Physics Publishing Electronic Journals* (37 titles) and by a substantial number of permanently or temporarily free journals available on the Net. A survey conducted by the Library among the readers on the usage of e-journals revealed that many researchers want access to as many titles as possible. Moreover, the survey identified a need for additional education on the use of electronic information databases (<http://knjiznica.irb.hr/eng/anketa/index.html>)

Regular monthly IRB Library Colloquia were held on "hot" issues about information sciences and librarianship. All this discussions, with their presentations, can be found at the address <http://knjiznica.irb.hr/eng/kolokviji.html>

The staff of the Library took active part in numerous meetings and conferences at home and abroad. They also attended organised seminars and workshops.

We have cooperated closely with libraries in Croatia and abroad. Cooperation with Information Center of American Embassy in Zagreb, central libraries of Croatian Science Information System, Universitätsbibliothek Regensburg (joint project ElektronischeZeitschriftenDatenbank), Central Engineering Library in Ljubljana, University Library in Maribor and Universitätsbibliothek Bochum, should be emphasized.

The regularly maintained web portal (<http://library.irb.hr>) has about 2500 pages. As the maintenance of such a great number of static pages is a very demanding task, we are planning to urgently make a new dynamic web. We would like to point out that apart from developing and maintaining the Library's web pages, we provide the following services:

- the web pages *Science on the Internet* (<http://znanost.irb.hr>) offer relevant information sources on specific scientific fields (Physics, Chemistry, Mathematics, Biology, Medicine, Earth Sciences, Environment, Computing and Librarianship)
- information about most outstanding Croatian scholars (<http://library.irb.hr/scientist/index.html>) with assorted web resources with numerous biographic and bibliographic data, photographs etc;
- Croatian press (<http://library.irb.hr/hrtis.html>) with links to daily papers, weekly journals and other publications;
- electronic versions of the Institute's annual reports, starting in the year 1993 (<http://knjiznica.irb.hr/izvjestaj/>);
- virtual reference library: numerous dictionaries, encyclopaedias and handbooks on natural sciences (<http://library.irb.hr/vrl/index.html>);
- information on electronic resources available to users (<http://library.irb.hr/resources.html>);

-Libraries in Croatia (<http://library.irb.hr/crolibs.html>) – a survey of about 140 Croatian libraries on the Web with links to their online catalogues.

-a list of CD-ROMs (<http://library.irb.hr/listacd.html>)

The library of the future we see as a comprehensive information centre where users will have access to all relevant information sources and to high quality education. The library of the future we see as fully aware of its role and responsibility towards coming generations. In this respect we will advocate the integrity of library collections. By modernisation of such segments of library management, as acquiring, processing, lending etc, we will secure resources for new tasks, such as efficient retrieval and dissemination of information, development of digital libraries, evaluation of web information sources, electronic publishing etc. In the future we plan a stronger international co-operation, participating in international projects, as well as involving foreign experts in domestic projects.

## **COMPUTING CENTRE**

Head of the Center: Ph. D. Karolj Skala

### **Research programme:**

Advancement, development and maintenance of the Institute's computers, computer network and services. The activities include server computers for information services, numerical computation on the computer cluster, printing, plotting, e-mail, web etc., as well as the Institute's local area network and network equipment which connects the personal and server computers on all the Institute divisions and laboratories. Maintenance of the network services, software implementation and development, and other activities related to the advancement of computer usage in scientific work (the development of e-science technology). Carrying out the scientifically applied and development projects in the field of modern network technology, distributed computing, cluster computing and GRID systems. Maintaining the scientific and technological cooperation with other scientific and business institutions, as well as CARNet.

The most important results of the Computing Centre are: design and partial implementation of the new computer network; development of a new type of hybrid SM/MM fiber-optic cables; development of laser-based transfer of data through atmosphere; enhancement of the computer cluster, and the CRO GRID initiative of a complex technology project with eight institutions.

Initiating an international collaboration on the project initiation and execution.

### **LOCAL AREA NETWORK CONSTRUCTION IN THE INSTITUTE**

Head of the Project: Ph. D. Karolj Skala

### **FREE SPACE LASER COMMUNICATION SYSTEM FOR DATA TRANSMISSION**

Head of the Project: Ph. D. Karolj Skala

### **NETWORK MONITORING AND MANAGEMENT OF THE CLUSTER COMPUTERS**

Head of the Project: Ph. D. Karolj Skala

### **DEVELOPMENT OF NEW GRID TECHNOLOGIES FOR ADVANCED SCIENTIFIC AND ENGINEERING APPLICATION**

Head of the Project: Ph. D. Karolj. Skala